# Microwave Spectra of Molecules of Astrophysical Interest
# VII. Carbon Monoxide, Carbon Monosulfide, and Silicon Monoxide

**Frank J. Lovas and Paul H. Krupenie**

*Institute for Basic Standards, National Bureau of Standards, Washington, D.C. 20234*

The available data on the microwave spectra of carbon monoxide, carbon monosulfide, and silicon monoxide are critically reviewed for information applicable to radio astronomy. Molecular data such as rotational constants, centrifugal distortion parameters, dipole moments, hyperfine coupling constants, and structure are tabulated. Observed rotational transitions are presented for all measured isotopic forms of these molecules. All of the available data has been analyzed in order to predict all rotational transitions of these molecules up to 300 GHz. Error limits have been taken from the original literature for each measured transition frequency. All predicted transition frequencies are given with estimated uncertainties which represent the 90 percent confidence limit.

Key words: Carbon monoxide; carbon monosulfide; interstellar molecules; microwave spectra; molecular parameters; radio astronomy; rotational transitions; silicon monoxide.

## Contents

## 1. Introduction

The present tables are part of a series of critical reviews [1–6][1] on the rotational spectra of molecules already identified in the interstellar medium. All of the available data have been gathered for each molecule and subjected to reanalysis in order to provide a consistent set of molecular constants, a check on the reliability of the measured transitions, and allow the unobserved transitions to be predicted with known uncertainty limits. Thus, the spectroscopic information presented in the following tables includes predicted as well as observed transitions in the frequency range presently accessible to the radio telescopes. The only limit invoked in the present calculations is a restriction on the maximum calculated frequency to approximately 300 GHz, which is more than sufficient to cover the frequency range of existing radio telescopes.

For the less abundant isotopic species of the molecules reported there are usually insufficient data to present a comprehensive statistical analysis of the spectrum. In these instances, reliable calculational techniques are invoked whereby molecular constants

---

[1] Numbers in brackets indicate references in section 1.2.

245

**J. Phys. Chem. Ref. Data, Vol. 3, No. 1, 1974**

necessary for predicting the spectrum can be determined. Details will be given in the discussion of each analysis separately. This review covers all the applicable information as of September, 1973.

A full description of the theory of rotational spectra is given in a number of texts, but the discussions by Townes and Schawlow [7] and Gordy and Cook [8] are particularly useful and the notation used here is generally consistent with these texts. The present analysis utilizes the Dunham [9] nomenclature as well as the usual spectroscopic formulation for describing the molecular parameters and energy level expressions. A general Dunham formulation of the equations for calculating the transition frequencies is

$$\nu_v = 2J\left[Y_{01} + Y_{11}(v+\tfrac{1}{2}) + Y_{21}(v+\tfrac{1}{2})^2\right]$$
$$+ 4J^3\left[Y_{02} + Y_{12}(v+\tfrac{1}{2})\right] + (6J^5 + 2J^3)Y_{03}. \quad (1)$$

The equivalent formulation in terms of the traditional spectroscopic constants is

$$\nu_v = 2JB_v - 4J^3 D_v + (6J^5 + 2J^3)H_v \quad (2)$$

where $B_v = B_e - \alpha_e(v+\tfrac{1}{2}) + \gamma_e(v+\tfrac{1}{2})^2$ and $D_v = D_e + \beta_e$ $(v+\tfrac{1}{2})$. Here $J$ represents the rotational quantum number of the upper state involved in the transition, $v$ is the vibrational quantum number, and $\nu$ is the transition frequency. The $Y_{ij}$ are related to the traditional spectroscopic constants and are proportional to the reduced mass of the molecules as follows:

$$Y_{01} \cong B_e \propto 1/\mu_r \quad (3a)$$

$$Y_{11} \cong -\alpha_e \propto 1/\mu_r^{3/2} \quad (3b)$$

$$Y_{21} \cong \gamma_e \propto 1/\mu_r^2 \quad (3c)$$

$$Y_{02} \cong -D_e \propto 1/\mu_r^2 \quad (3d)$$

$$Y_{12} \cong -\beta_e \cong 1/\mu_r^{5/2} \quad (3e)$$

$$Y_{03} \cong H_e \propto 1/\mu_r^3 \quad (3f)$$

where $\mu_r = M_1 M_2/(M_1 + M_2)$ with $M_1$ and $M_2$ referring to the masses of the two atoms composing the molecule. A further generalized relation which is employed in calculations for CS and SiO is known as the Kratzer relation [10]:

$$-Y_{02} = D_e = 4B_e^3/\omega_e^2 \quad (4)$$

where $\omega_e$ is the equilibrium vibrational constant for the molecule. For diatomic molecules where $\omega_e$ is sufficiently well known, this relation has been shown to be accurate to better than 1 percent.

For all of the analyses described in this review, the least squares fitting was performed utilizing a weighting

factor. This weight was equal to the inverse square of the measured uncertainty. The hyperfine structure calculations were based on the usual expression:

$$-eqQ f(I, J, F) + \tfrac{1}{2} c[F(F+1)$$
$$- J(J+1) - I(I+1)] \quad (5)$$

where $f(I, J, F)$ is the Casimir function. The values of the Casimir function as well as the calculated relative intensities for the hyperfine components can be found in Appendix I of [7]. The standard deviations quoted for both the molecular constants and predicted frequencies were selected to represent the 90 percent confidence limit. For a number of the less abundant isotopic forms, where only one transition frequency has been measured, the uncertainty in the measurement was assumed to be one standard deviation. This estimated standard deviation was then utilized in calculating the uncertainties for the predicted transitions.

Following the method of the sixth paper in this series, the present tables do not include line strengths other than the relative intensities of the nuclear electric quadrupole split transitions. The line strength, $S$, is a simple function of the quantum numbers as follows:

$$S(J'; J'') = J'$$

The Einstein coefficient, $A(J'; J'')$, which is the probability of a spontaneous transition in one second from the upper state, $J'$, to the lower state, $J''$, is given by

$$A(J'; J'') = \frac{1.1639 \times 10^{-20}\nu^3\mu^2}{2J'+1} S(J'; J'')$$

where $\mu$ is the dipole moment in Debye and $\nu$ is the transition frequency in MHz.

### 1.1. List of Symbols and Conversion Factors

#### a. Symbols

$Y_{ij}$    Dunham coefficients in the power series expansion for the rotational and vibrational energy expression. (See text).

$B_v, B_e$    Rotational constant for the $v$th vibrational state $(B_v)$ and at the equilibrium internuclear distance $(B_e)$ respectively.

$$B_e = \frac{\hbar}{4\pi\mu_r r_e^2} \text{ [MHz]}$$

$D_v, D_e$    Centrifugal distortion (quartic) constant. (kHz or MHz).

$H_v$    Sextic distortion constant. (Hz).

$eqQ$    Nuclear electric quadrupole coupling constant (MHz).

$c_X$    Spin-rotation constant related to nucleus X.

$J$    Total rotational angular momentum quantum number.

$F$    Total angular momentum quantum number which includes the nuclear spin for the nucleus with largest $eqQ$.

$I$    Nuclear spin angular momentum quantum number.

$\mu_v$    Dipole moment of the molecule in the $v$th vibrational state (Debye).

$v$    Vibrational quantum number.

$\mu_r$    Reduced mass (amu).

(...)    Parentheses in the numerical listings contain measured or estimated uncertainties. These should be interpreted as: $1.409(0.083) = 1.409(83) = 1.409 \pm 0.083$ MHz.

and"    Prime and double prime. Superscripts to the quantum number indicators which refer to the upper and lower energy state, respectively.

### b. Conversion Factors

$$Y_{01} \cong B_e \text{ (MHz)} = \frac{5.05376 \times 10^5}{\mu_r r_e^2 \text{ (amu Å}^2)}.$$

$$1 \text{ cm}^{-1} = 29{,}979.2458 \text{ MHz }^2$$

### 1.2. References

[1] D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff, J. Phys. Chem. Ref. Data 1, 1011 (1972).

[2] W. H. Kirchhoff, D. R. Johnson, and F. J. Lovas, J. Phys. Chem. Ref. Data 2, 1 (1973).

[3] R. M. Lees, F. J. Lovas, W. H. Kirchhoff, and D. R. Johnson, J. Phys. Chem. Ref. Data 2, 205 (1973).

[4] P. Helminger, F. C. DeLucia, and W. H. Kirchhoff, J. Phys. Chem. Ref. Data 2, 215 (1973).

[5] F. C. DeLucia, P. Helminger and W. H. Kirchhoff, J. Phys. Chem. Ref. Data 2,     (1973).

[6] A. G. Maki, J. Phys. Chem. Ref. Data, 3,     (1974).

[7] C. H. Townes and A. L. Schawlow, Microwave Spectroscopy, McGraw-Hill, New York, 1955.

[8] W. Gordy and R. L. Cook, Microwave Molecular Spectra, John Wiley & Sons, New York. 1970.

[9] J. L. Dunham, Phys. Rev. 41, 721 (1932).

[10] A. Kratzer, Z. Phys. 3, 289 (1920).

## 2. Carbon Monoxide

The rotational constants and other pertinent molecular parameters are given in table 1. The most extensive data available exist for $^{12}C^{16}O$, which requires only two

---

² In keeping with the commonly accepted convention in molecular spectroscopy, the fundamental frequencies and vibrational energies are frequently expressed in their wavenumber (cm⁻¹) equivalents. The actual frequency in units of hertz may be obtained by multiplying the numbers in such tables by the speed of light expressed in centimeters per second. Energies are obtained by multiplying the frequencies by Planck's constant.

parameters for fitting, namely, $B_0$ and $D_0$ of eq (2). Since only the lowest transition, the $J = 1 \leftarrow 0$, has been measured for the other isotopic species, the centrifugal distortion parameter, $D_0$, had to be calculated indirectly. Here the isotopic mass dependence of $D_0$ as given in eq (3d) was employed. The $D_0$ values for all less abundant isotopic species were calculated from the $D_0$ value of $^{12}C^{16}O$, and the higher frequency transitions for the less abundant isotopic species were calculated from the equation:

$$\nu^i_{J'-J''} = J'(\nu^i_{1 \leftarrow 0}) - 4D^i_0(J'^3 - J') \qquad (6)$$

for $J' \geqslant 2$ where $\nu^i_{1 \leftarrow 0}$ is the transition frequency for $J = 1 \leftarrow 0$ of the $i$th isotopic species. Because of the known breakdown in the Born-Oppenheimer approximation, which is assumed in deriving the isotopic relations given in the introduction, this technique for calculating the transition frequencies is more reliable than applying the isotope relations to $B_0$. The uncertainty introduced by calculating the centrifugal distortion for the less abundant isotopic species from these isotopic relations is of the order of one part in ten thousand and, thus, relatively small in absolute terms. The uncertainties quoted for the $^{12}C^{16}O$ calculated transition frequencies in table 2 are two standard deviations, i.e., approximately 90 percent confidence limit.

Since only one measurement exists for each of the less abundant isotopic species shown in tables 3–7, it is difficult to determine the meaning of the standard deviation uncertainties quoted in terms of confidence limit. In the present analysis the reported uncertainty for the measured transition was assumed to be one standard deviation. Our experience has shown this to be generally the case. In an attempt to report the 90 percent confidence limit, three times this standard deviation was chosen.

### 2.1. Organization of the Spectral Tables

Tables 2 through 7 contain the rotational quantum numbers, $J$, in the first two columns. These are followed by the observed transition frequency in MHz in the third column and the calculated frequency in MHz in the fourth column. Associated with each observed or calculated frequency is the estimated uncertainty, shown in parentheses, which refers to the last digits given. The fifth column contains the upper state energy in cm⁻¹ units. The last column lists the references for the observed transitions. For the convenience of the user, the transition frequencies given in tables 2–7 are listed according to increasing frequency in table 8.

## 2.2. Carbon Monoxide Spectral Tables

Table 1.   Molecular constants for Carbon Monoxide.

| Isotopic Species | $B_0$ (MHz) | $D_0$ (kHz) | Ref. |
|---|---|---|---|
| $^{12}C^{16}O$ | 57635.9687(26) | 183.567(70) | a |
| $^{12}C^{17}O$ | 56179.9828(252) | 174.388(100) | 57B[b] |
| $^{12}C^{18}O$ | 54891.4239(122) | 166.462(95) | 58A[b] |
| $^{13}C^{16}O$ | 55101.0205(122) | 167.745(96) | 58A[b] |
| $^{13}C^{18}O$ | 52356.0108(122) | 151.405(87) | 58A[b] |
| $^{14}C^{16}O$ | 52935.8646(122) | 154.786(87) | 58A[b] |

Dipole Moment for $^{12}C^{16}O$

$$\mu_0 = 0.112(5) \ [D] \qquad 58B$$

Hyperfine structure constants for $^{12}C^{17}O$

$$eq_0Q \ (^{17}O) = 4.52(69) \ [MHz]$$

$$c \ (^{17}O) = 24.6(106) \ [kHz]$$

[a]Refit to data from [57A, 58A and 70A].

[b]The $J = 1 \leftarrow 0$ transition frequencies from the references given were used in determining the $B_0$ values given.  Note that $D_0$ was obtained from $^{12}C^{16}O$ value by the isotope relation, $D \propto \mu_r^{-2}$. All errors are 1 standard deviation.

Table 2.   The microwave spectrum of $^{12}C^{16}O$ (MHz).

| Transition Upper State J' | Lower State J" | Observed Frequency (Est. Unc.) | Calculated Frequency (Est. Unc.)[b] | Energy Levels in $cm^{-1}$ Upper State | Ref. |
|---|---|---|---|---|---|
| 1 | - 0 | 115271.204(5) | 115271.203(5) | 3.845 | 58A |
| 2 | - 1 | 230537.974(30) | 230538.001(9) | 11.535 | 57A |
| 3 | - 2 | 345795.989(100)[a] | 345795.987(13) | 23.069 | 70A |
| 4 | - 3 | 461040.811(100)[a] | 461040.756(19) | 38.448 | 70A |
| 5 | - 4 | 576267.934(100)[a] | 576267.903(31) | 57.670 | 70A |
| 6 | - 5 | 691472.978(100)[a] | 691473.022(52) | 80.735 | 70A |
| 7 | - 6 | 806651.719(100)[a] | 806651.707(83) | 107.642 | 70A |

[a]Uncertainty estimated for weighting in the least squares fit.

[b]In an attempt to estimate the 90% confidence limit two standard deviations are reported.

Table 3.  The microwave spectrum of $^{12}C^{17}O$ (MHz).

| Transition Upper State J' | - | Lower State J" | Observed Frequency (Est. Unc.) | Calculated Frequency (Est. Unc.)[a] | Relative Intensity | Energy Levels in cm$^{-1}$ Upper State | Ref. |
|---|---|---|---|---|---|---|---|
| 1 | - | 0 | | 112359.268(71) | | 3.748 | |
| F = 3/2 | - | F = 5/2 | 112358.72(10) | 112358.720(118) | [0.222] | | 57B |
| F = 7/2 | - | F = 5/2 | 112358.980(15) | 112358.981(100) | [0.444] | | 57B |
| F = 5/2 | - | F = 5/2 | 112360.016(15) | 112360.016(90) | [0.333] | | 57B |
| 2 | - | 1 | | 224714.351(142) | | 11.244 | |
| F = 3/2 | - | F = 5/2 | | 224713.51(24) | [0.040] | | |
| F = 5/2 | - | F = 5/2 | | 224714.00(16) | [0.122] | | |
| F = 7/2 | - | F = 5/2 | | 224714.14(15) | [0.171] | | |
| F = 9/2 | - | F = 7/2 | | 224714.19(15) | [0.333] | | |
| F = 1/2 | - | F = 3/2 | | 224714.71(16) | [0.067] | | |
| F = 3/2 | - | F = 3/2 | | 224714.71(15) | [0.093] | | |
| F = 5/2 | - | F = 7/2 | | 224715.03(18) | [0.016] | | |
| F = 7/2 | - | F = 7/2 | | 224715.17(20) | [0.095] | | |
| F = 5/2 | - | F = 3/2 | | 224715.29 (22) | [0.171] | | |
| 3 | - | 2 | | 337061.063(210) | | 22.487 | |
| F = 3/2 | - | F = 5/2 | | 337060.38(26) | [0.011] | | |
| F = 1/2 | - | F = 3/2 | | 337060.59(24) | [0.011] | | |
| F = 5/2 | - | F = 7/2 | | 337060.70(24) | [0.008] | | |
| F = 5/2 | - | F = 5/2 | | 337060.84(22) | [0.066] | | |
| F = 9/2 | - | F = 7/2 | | 337060.93(21) | [0.194] | | |
| F = 3/2 | - | F = 3/2 | | 337060.96(22) | [0.055] | | |
| F =11/2 | - | F = 9/2 | | 337060.95(21) | [0.286] | | |
| F = 7/2 | - | F = 7/2 | | 337061.04(21) | [0.065] | | |
| F = 1/2 | - | F = 1/2 | | 337061.14(21) | [0.037] | | |
| F = 7/2 | - | F = 5/2 | | 337061.18(21) | [0.122] | | |
| F = 5/2 | - | F = 3/2 | | 337061.10(22) | [0.069] | | |
| F = 3/2 | - | F = 1/2 | | 337061.51(22) | [0.030] | | |
| F = 9/2 | - | F = 9/2 | | 337061.91(25) | [0.044] | | |
| F = 7/2 | - | F = 9/2 | | 337062.02(26) | [0.004] | | |

[a]The three standard deviations reported are expected to approximate the 90% confidence limit.

Table 4.  The microwave spectrum of $^{12}C^{18}O$ (MHz).

| Transition | | | Observed Frequency | Calculated Frequency | Energy Levels | |
|---|---|---|---|---|---|---|
| Upper State | - | Lower State | (Est. Unc.) | (Est. Unc.) | in cm$^{-1}$ | Ref. |
| J' | - | J" | | | Upper State | |
| 1 | - | 0 | 109782.182(8) | 109782.182(24)[a] | 3.662 | 58A |
| 2 | - | 1 | | 219560.369(50) | 10.986 | |
| 3 | - | 2 | | 329330.566(81) | 21.971 | |

[a]The uncertainty assigned is 3 times that of the measured frequency. Under the assumption that the measuement uncertainty is one standard deviation, the calculated uncertainties represent the 90% confidence limit.

Table 5.  The microwave spectrum of $^{13}C^{16}O$ (MHz).

| | | | Observed Frequency | Calculated Frequency | Energy Levels | |
|---|---|---|---|---|---|---|
| Up,er State | - | Lower State | (Est. Unc.) | (Est. Unc.) | in cm$^{-1}$ | Ref. |
| J' | - | J" | | | Upper State | |
| 1 | - | 0 | 110201.370(8) | 110201 370(24)[a] | 3.676 | 58A |
| 2 | - | 1 | | 220398.714(50) | 11.028 | |
| 3 | - | 2 | | 330588.006(81) | 22.055 | |

[a]The uncertainty assigned is 3 times that of the measured frequency. Under the assumption that the measurement uncertainty is one standard deviation, the calculated uncertainties represent the 90% confidence limit.

Table 6.  The microwave spectrum of $^{13}C^{18}O$ (MHz).

| Transition | | | Observed Frequency | Calculated Frequency | Energy Levels | |
|---|---|---|---|---|---|---|
| Upper State | - | Lower State | (Est. Unc.) | (Est. Unc.) | in cm$^{-1}$ | Ref. |
| J' | - | J" | | | Upper State | |
| 1 | - | 0 | 104711.416(8) | 104711.416(24)[a] | 3.493 | 58A |
| 2 | - | 1 | | 209419.198(50) | 10.478 | |
| 3 | - | 2 | | 314119.713(80) | 20.956 | |

[a]The uncertainty assigned is 3 times that of the measured frequency. Under the assumption that the measurement uncertainty is one standard deviation, the calculated uncertainties represent the 90% confidence limit.

Table 7.  The microwave spectrum of $^{14}C^{16}O$ (MHz).

| Transition | | | Observed Frequency | Calculated Frequency | Energy Levels | |
|---|---|---|---|---|---|---|
| Upper State | - | Lower State | (Est. Unc.) | (Est. Unc.) | in cm$^{-1}$ | Ref. |
| J' | - | J" | | | Upper State | |
| 1 | - | 0 | 105871.110(4) | 105871.110(24)[a] | 3.531 | 58A |
| 2 | - | 1 | | 211738.505(50) | 10.594 | |
| 3 | - | 2 | | 317598.471(80) | 21.188 | |

[a]The uncertainty assigned is 6 times that of the measured frequency. Under the assumption that the measurement uncertainty is one standard deviation, the calculated uncertainties represent the 90% confidence limit.

Table 8.   Calculated microwave transitions in CO

in order of frequency (MHz).

| Calculated Frequency | Isotopic Species | Transition J' - J" | | Estimated Uncertainty |
|---|---|---|---|---|
| 104711.416 | $^{13}C^{18}O$ | 1 | - 0 | (0.024) |
| 105871.110 | $^{14}C^{16}O$ | 1 | - 0 | (0.024) |
| 109782.182 | $^{12}C^{18}O$ | 1 | - 0 | (0.024) |
| 110201.370 | $^{13}C^{16}O$ | 1 | - 0 | (0.024) |
| 112359.268 | $^{12}C^{17}O$ | 1 | - 0 | (0.071) |
| 115271.203 | $^{12}C^{16}O$ | 1 | - 0 | (0.005) |
| 209419.198 | $^{13}C^{18}O$ | 2 | - 1 | (0.050) |
| 211738.505 | $^{14}C^{16}O$ | 2 | - 1 | (0.050) |
| 219560.369 | $^{12}C^{18}O$ | 2 | - 1 | (0.050) |
| 220398.714 | $^{13}C^{16}O$ | 2 | - 1 | (0.050) |
| 224714.351 | $^{12}C^{17}O$ | 2 | - 1 | (0.142) |
| 230538.001 | $^{12}C^{16}O$ | 2 | - 1 | (0.009) |
| 314119.713 | $^{13}C^{18}O$ | 3 | - 2 | (0.080) |
| 317598.471 | $^{14}C^{16}O$ | 3 | - 2 | (0.080) |
| 329330.566 | $^{12}C^{18}O$ | 3 | - 2 | (0.081) |
| 330588.006 | $^{13}C^{16}O$ | 3 | - 2 | (0.081) |
| 337061.063 | $^{12}C^{17}O$ | 3 | - 2 | (0.210) |
| 345795.987 | $^{12}C^{16}O$ | 3 | - 2 | (0.013) |
| 461040.756 | $^{12}C^{16}O$ | 4 | - 3 | (0.019) |
| 576267.903 | $^{12}C^{16}O$ | 5 | - 4 | (0.031) |
| 691473.022 | $^{12}C^{16}O$ | 6 | - 5 | (0.052) |
| 806651.707 | $^{12}C^{16}O$ | 7 | - 6 | (0.083) |

## 2.3. CO References

### a. Laboratory References

[50A] Gilliam, O. R., Johnson, C. M., and Gordy, W., "Microwave spectrum in the region from 2–3 mm.", Phys. Rev. 78, 140 (1950).

[53A] Bedard, F. D., Gallagher, J. J., and Johnson, C. M., "Microwave measurement of $D_0$ for CO.", Phys. Rev. 92, 1440 (1953).

[56A] Cowan, M., and Gordy, W., "Further extension of microwave spectroscopy in the submillimeter-wave region", Phys. Rev. 104, 551 (1956).

[56B] Cox, J. T., and Gordy, W., "Zeeman effect of some linear and symmetric-top molecules", Phys. Rev. 101, 1298 (1956).

[57A] Gordy, W., and Cowan, M. J., "Precision measurement of millimeter and submillimeter wave lines of CO", Bull. Amer. Phys. Soc. 2, 212 (1957).

[57B] Rosenblum, B., and Nethercot, A. H., Jr., "Quadrupole coupling constant and molecular structure of $CO^{17}$", J. Chem. Phys. 27, 828 (1957).

[58A] Rosenblum, B., Nethercot, A. H., and Townes, C. H., "Isotopic mass ratios, magnetic moments and the sign of the electric dipole moment in carbon monoxide", Phys. Rev. 109, 400 (1958).

[58B] Burrus, C. A., "Stark effect from 1.1 to 2.6 mm wavelength: $PH_3$, $PD_3$, DI, CO", J. Chem. Phys. 28, 427 (1958).

[59A] Burrus, C. A., "Zeeman effect in the 1- to 3-millimeter wave region: Molecular g factors of several light molecules", J. Chem. Phys. 30, 976 (1959).

[64A] Jones, G., and Gordy, W., "Extension of submillimeter-wave spectroscopy below a half-millimeter wavelength", Phys. Rev. 135A, 295 (1964).

[66A] Flygare, W. H., and Weiss, V. W., "$^{13}C$ spin-rotation interaction and magnetic shielding at the carbon and oxygen nuclei in formaldehyde", J. Chem. Phys. 45, 2785 (1966).

[67A] Ozier, I., Yi, P., Khosla, A., and Ramsey, N. F., "Sign and magnitude of the rotational moment of $^{12}C^{16}O$", J. Chem. Phys. 46, 1530 (1967).

[68A] Ozier, I., Crapo, L. M., and Ramsey, N. F., "Spin rotation constant and rotational magnetic moment of $^{13}C^{16}O$", J. Chem. Phys. 49, 2314 (1968).

[70A] Helminger, P., DeLucia, F. C., and Gordy, W., "Extension of microwave absorption spectroscopy to 0.37 mm wavelength", Phys. Rev. Lett. 25, 1397 (1970).

### b. Interstellar References

Wilson, R. W., Jefferts, K. B., and Penzias, A. A., "Carbon monoxide in the Orion nebula", Astrophys. J. 161, L43 (1970).

Solomon, P., Jefferts, K. B., Penzias, A. A., and Wilson, R. W., "Observation of CO emission at 2.6 millimeter from IRC+10216", Astrophys. J. 163, L53 (1971).

Penzias, A. A., Jefferts, K. B., and Wilson, R. W., "Interstellar $^{12}C^{16}O$, $^{13}C^{16}O$ and $^{12}C^{18}O$", Astrophys. J. 165, 229 (1971).

Wilson, R. W., Solomon, P. M., Penzias, A. A., and Jefferts, K. B., "Millimeter observations of CO, CN, and CS emission from IRC+10216", Astrophys. J. 169, L35 (1971).

Penzias, A. A., Solomon, P. M., Jefferts, K. B., and Wilson, R. W., "Carbon monoxide observations of dense interstellar clouds", Astrophys. J. 174, L43 (1972).

Schwartz, P. R., and Wilson, W. J., "A search for interstellar $^{14}CO$", Astrophys. J., 177, L129 (1972).

Solomon, P. M., Scoville, N. Z., Jefferts, K. B., Penzias, A. A., and Wilson, R. W., "Molecular clouds in the galactic center region: Carbon monoxide observations at 2.6 millimeters", Astrophys. J. 178, 125 (1972).

Penzias, A. A., Jefferts, K. B., Wilson, R. W., Liszt, H. S., and Solomon, P. M., "$^{13}C^{16}O/^{12}C^{18}O$ ratios in nine H I regions", Astrophys. J. 178, L35 (1972).

Wilson, W. J., Schwartz, P. R., and Epstein, E. E., "Carbon monoxide and hydrogen cyanide millimeter-wave emission from stars", Astrophys. J. 183, 871 (1973).

Loren, R. B., Vander Bout, P. A., and Davis, J. H., "Carbon monoxide emission from nebulosity associated with Herbig $B_e$ and $A_e$ type stars", Astrophys. J. 185, L67 (1973).

Schwartz, P. R., Wilson, W. J., and Epstein, E. E., "The distribution of galactic carbon monoxide: A preliminary survey", Astrophys. J. 186, 529 (1973).

Tucker, K. D., Kutner, M. L., and Thaddeus, P., "A large carbon monoxide cloud in Orion", Astrophys. J. 186, L13 (1973).

Phillips, T. G., Jefferts, K. B., and Wannier, P. G., "Observation of the J=2 to J=1 transition of interstellar CO at 1.3 millimeters", Astrophys. J. 186, L19 (1973).

Jefferts, K. B., Penzias, A. A., and Wilson, R. W., "Interstellar oxygen-17", Astrophys. J. 186, L77 (1973).

## 3. Carbon Monosulfide

The present reanalysis of the rotational spectrum of $^{12}C^{32}S$ and $^{12}C^{34}S$ differs from that given in the most

recent source of data [63A] in that we find $B_0$ and $D_0$ as the determinable parameters. In [63A], the parameters $B_0$, $D_0$ and $H_0$ from eq (2) were used in fitting the available data. The present analysis shown in table 9 utilizes only $B_0$ and $D_0$, since it was concluded that $H_0$ was not a determinable constant. The standard deviation errors shown represent the 90 percent confidence limit.

In the case of $^{12}C^{32}S$ where five of the six rotational transitions have been measured, a least squares fit which includes $H_0$ produced the following constants:

$$B_0 = 24495.586(5) \text{ MHz,}$$
$$D_0 = \quad 42.18(70) \text{ kHz,}$$
$$H_0 = \quad 50.54(18) \text{ Hz,}$$

quoting two standard deviation errors. Here the magnitude of $H_0$ seems much greater than expected from several points of view. First of all, a generally applicable approximation: $D_e/H_e \cong \omega_e^2/B_e^2 = 10^6$ indicates that $H_0$ should be 0.04 Hz rather than 50 Hz. In addition, there is another approximation for estimating $H_e$ from the value of $\alpha_e$:

$$H_e = -8/3\,(B_e^3/\omega_e^3)\,\alpha_e + 32\,B_e^5/\omega_e^4.$$

Since the $J = 1 \leftarrow 0$, $v = 1$ transition for $^{12}C^{32}S$ has been measured, $\nu = 48635.912(40)$, a value of $\alpha_e = 177.54(3)$ [55A], can be determined and thereby $H_e$ is estimated from the above relation to be $+ 0.01$ Hz. Values of $H_0$ of this magnitude would contribute less than 2 kHz to the $J = 5\text{-}4$ transition, two orders of magnitude smaller than the measurement uncertainty. A further point of comparison is possible. Since three transitions of $^{12}C^{34}S$ have been observed, $B_0$ and $D_0$ can be derived with reasonable accuracy. Via the isotope relation, eq (3d), applied to $D_0$ for $^{12}C^{32}S$, a value of $D_0$ ($^{12}C^{34}S$) $= 34.96(54)$ kHz is obtained. This $D_0$ value agrees well with that derived for $^{12}C^{34}S$ from the transition frequencies as shown

in table 9 where the six standard deviation error shown represent the 90 percent confidence limit. In order to make the final comparison, an over-determined fit of three parameters $B_0$, $D_0$ and $H_0$, to the three transitions was carried out with the results

$$B_0 = 24103.553 \text{ MHz,}$$
$$D_0 = \quad 39.792 \text{ kHz,}$$
$$H_0 = \quad 62.5 \text{ Hz,}$$

wherein no estimated uncertainty can be given due to zero degrees of freedom in the fit. Note that not only is $H_0$ again unreasonably large, but $D_0$ is calculated 1 kHz larger than the two calculations described above. For these reasons the $H_0$ values appear to be misleading and undeterminable from the data available.

Calculations of the remaining two isotopic species of CS, namely $^{12}C^{33}S$ and $^{13}C^{32}S$ followed the procedure employed for most of the CO calculations. Since only the $J = 1\text{-}0$ transitions have been observed, $D_0$ was computed via the isotope relations. The transition frequencies were then calculated according to eq (6) in order to minimize the estimated uncertainties. Since the hyperfine structure calculation was overdetermined for $^{12}C^{33}S$ following eq (5), the quoted uncertainties are four standard deviations while those for $^{13}C^{32}S$ are two standard deviations. All uncertainties are expected to represent the 90 percent confidence limit.

### 3.1. Organization of the Spectral Tables

Following the format of the CO tables as well as those of earlier reviews in this series, the format of tables 10 through 13 contain, first the quantum numbers, then the observed transition frequency, the calculated frequency and estimated uncertainty in parentheses, the energy of the upper state and finally references to measurements. Table 14 contains all the CS transitions up to 300 GHz, listed according to increasing frequency.

## 3.2. Carbon Monosulfide Spectral Tables

Table 9.  Molecular constants for Carbon Monosulfide.

| Constant[a] | $^{12}C^{32}S$ | $^{12}C^{33}S$ | $^{12}C^{34}S$ | $^{13}C^{32}S$ |
|---|---|---|---|---|
| $B_0$ (MHz) | 24495.5746(102) | 24293.3390(63) | 24103.5507(121) | 23123.808(20) |
| $D_0$ (kHz) | 40.237(568) | 39.574(559)[b] | 38.774(776) | 35.849(506)[b] |
| eqQ [$^{33}$S] (MHz) | | 12.835(33) | | |
| $c_S$ (kHz) | | 18.7(37) | | |
| $\mu_0$ (Debye) | 1.958(5)[c] | | | |

[a]The constants were derived from the data in references [63A] and [55A] unless otherwise indicated. $^{12}C^{32}S$: Uncertainty in $B_0$ and $D_0$ represents 2 standard deviation, based on a least squares fit with 3 degrees of freedom; uncertainty in $\mu_0$ is 1 standard deviation. $^{12}C^{33}S$: Uncertainty in $B_0$ and $D_0$ represents 2 standard deviation; uncertainty in eqQ and $c_S$ represents 1 standard deviation; $^{12}C^{34}S$: Uncertainty in $B_0$ and $D_0$ represents 6 standard deviation, based on a least squares fit with 1 degree of freedom. $^{13}C^{32}S$: Uncertainty in $B_0$ and $D_0$ represents 2 standard deviation.

[b]Calculated from the $D_0$ value for $^{12}C^{32}S$ by use of the isotope relation.

[c]Reference [68A].

Table 10. The microwave spectrum of $^{12}C^{32}S$ (MHz).

| Transition | | Observed Frequency[a] | Calculated Frequency[b] | Energy Levels in cm$^{-1}$ | Ref. |
|---|---|---|---|---|---|
| Upper state J' | Lower state J" | (Est. Unc.) | (Est. Unc.) | Upper state | |
| 1 | 0 | 48991.000(12) | 48990.988(20) | 1.634 | 55A |
| 2 | 1 | 97981.007(16) | 97981.011(32) | 4.902 | 63A |
| 3 | 2 | 146969.039(60) | 146969.102(50) | 9.804 | 63A |
| 4 | 3 | 195954.162(100) | 195954.296(108) | 16.340 | 63A |
| 5 | 4 | 244935.737(100) | 244935.627(226) | 24.510 | 63A |
| 6 | 5 | | 293912.13(42) | 34.314 | |

[a]Estimated uncertainty represents 1 standard deviation.

[b]In an attempt to estimate the 90% confidence limit two standard deviations are reported.

Table 11. The microwave spectrum of $^{12}C^{33}S$ (MHz).

| Transition | | Observed Frequency[a] | Calculated Frequency[b] | Relative Intensity[c] | Energy Levels in cm$^{-1}$ | Ref. |
|---|---|---|---|---|---|---|
| Upper state J' | Lower state J" | (Est. Unc.) | (Est. Unc.) | | Upper State | |
| 1 | 0 | | 48586.5197(248) | | 1.621 | |
| F = 1/2 | F = 3/2 | 48583.264(10) | 48583.264(25) | [0.167] | | 55A |
| F = 5/2 | F = 3/2 | 48585.906(10) | 48585.906(25) | [0.500] | | 55A |
| F = 3/2 | F = 3/2 | 48589.068(10) | 48589.068(25) | [0.333] | | 55A |
| 2 | 1 | | 97172.090(56) | | 4.862 | |
| F = 1/2 | F = 3/2 | | 97166.239(100) | [0.017] | | |
| F = 3/2 | F = 3/2 | | 97169.486(68) | [0.107] | | |
| F = 5/2 | F = 3/2 | | 97171.824(56) | [0.210] | | |
| F = 7/2 | F = 5/2 | | 97171.843(60) | [0.400] | | |
| F = 1/2 | F = 1/2 | | 97172.053(64) | [0.083] | | |
| F = 3/2 | F = 5/2 | | 97172.648(80) | [0.010] | | |
| F = 5/2 | F = 5/2 | | 97175.042(66) | [0.090] | | |
| F = 3/2 | F = 1/2 | | 97175.289(66) | [0.083] | | |
| 3 | 2 | | 145755.760(130) | | 9.725 | |
| F = 3/2 | F = 3/2 | | 145753.137(140) | [0.040] | | |
| F = 5/2 | F = 5/2 | | 145754.054(140) | [0.052] | | |
| F = 7/2 | F = 5/2 | | 145755.617(132) | [0.245] | | |
| F = 9/2 | F = 7/2 | | 145755.635(132) | [0.359] | | |
| F = 3/2 | F = 1/2 | | 145756.374(132) | [0.100] | | |
| F = 5/2 | F = 3/2 | | 145756.392(132) | [0.160] | | |
| F = 7/2 | F = 7/2 | | 145758.760(140) | [0.041] | | |
| 4 | 3 | | 194336.582(286) | | 16.207 | |
| F = 5/2 | F = 5/2 | | 194333.543(294) | [0.023] | | |
| F = 7/2 | F = 7/2 | | 194335.285(292) | [0.030] | | |
| F = 9/2 | F = 7/2 | | 194336.495(286) | [0.255] | | |
| F =11/2 | F = 9/2 | | 194336.513(286) | [0.333] | | |
| F = 5/2 | F = 3/2 | | 194336.829(286) | [0.143] | | |
| F = 7/2 | F = 5/2 | | 194336.848(286) | [0.191] | | |
| F = 9/2 | F = 9/2 | | 194339.619(294) | [0.023] | | |
| 5 | 4 | | 242913.605(550) | | 24.310 | |
| F =11/2 | F = 9/2 | | 242913.547(550) | [0.258] | | |
| F =13/2 | F =11/2 | | 242913.566(550) | [0.318] | | |
| F = 7/2 | F = 5/2 | | 242913.730(550) | [0.167] | | |
| F = 9/2 | F = 7/2 | | 242913.748(550) | [0.207] | | |
| 6 | 5 | | 291485.879(950) | | 34.033 | |

# F. J. LOVAS AND P. H. KRUPENIE

Table 11.  The microwave spectrum of $^{12}C^{33}S$ (MHz)—Continued

| Transition | | Observed Frequency[a] | Calculated Frequency[b] | Relative | Energy Levels | Ref. |
|---|---|---|---|---|---|---|
| Upper state | Lower state | (Est. Unc.) | (Est. Unc.) | Intensity[c] | in cm$^{-1}$ | |
| $J'$ | $J''$ | | | | Upper State | |
| F =13/2 - | F =11/2 | | 291485.839(950) | [0.259] | | |
| F =15/2 - | F =13/2 | | 291485.858(950) | [0.308] | | |
| F = 9/2 - | F = 7/2 | | 291485.948(950) | [0.182] | | |
| F =11/2 - | F = 9/2 | | 291485.967(950) | [0.217] | | |

[a]Estimated uncertainty is approximately 1 standard deviation.

[b]Estimated uncertainty is 4 standard deviations, in an attempt to estimate the 90% confidence limit.

[c]With the exception of the J = 2 - 1 hyperfine structure calculations for which all allowed transitions are included, the calculated transitions were limited to those with relative intensities greater than 0.01 or one percent. The relative intensities are based on unity for each rotational transition J' - J".

Table 12.  The microwave spectrum of $^{12}C^{34}S$ (MHz).

| Transition | | Observed Frequency[a] | Calculated Frequency[b] | Energy Levels | Ref. |
|---|---|---|---|---|---|
| Upper state | Lower state | (Est. Unc.) | (Est. Unc.) | in cm$^{-1}$ | |
| $J'$ | $J''$ | | | Upper state | |
| 1 - | 0 | 48206.948(12) | 48206.946(22) | 1.608 | 55A |
| 2 - | 1 | 96412.953(30) | 96412.962(28) | 4.824 | 63A |
| 3 - | 2 | 144617.117(16) | 144617.116(32) | 9.648 | 63A |
| 4 - | 3 | | 192818.48(11) | 16.080 | |
| 5 - | 4 | | 241016.12(28) | 24.119 | |
| 6 - | 5 | | 289209.11(53) | 33.766 | |

[a]Estimated uncertainty represents 1 standard deviation.

[b]Estimated uncertainty represents 6 standard deviations, in an attempt to estimate the 90% confidence limit.

Table 13.  The microwave spectrum of $^{13}C^{32}S$ (MHz).

| Transition | | Observed Frequency[b] | Calculated Frequency[c] | Energy Levels | Ref. |
|---|---|---|---|---|---|
| Upper state | Lower state | (Est. Unc.) | (Est. Unc.) | in cm$^{-1}$ | |
| $J'$ | $J''$ | | | Upper state | |
| 1 - | 0 | 46247.472(20) | 46247.472(40)[a] | 1.543 | 55A |
| 2 - | 1 | | 92494.084(81) | 4.628 | |
| 3 - | 2 | | 138738.97(13) | 9.256 | |
| 4 - | 3 | | 184981.28(20) | 15.426 | |
| 5 - | 4 | | 231220.15(31) | 23.139 | |
| 6 - | 5 | | 277454.72(49) | 32.394 | |

[a]All predicted transition frequencies are based on this value, using the $D_0$ value from $^{12}C^{32}S$ and the isotope relations.

[b]Estimated uncertainty represents 1 standard deviation.

[c]Estimated uncertainty represents 2 standard deviations, in an attempt to estimate the 90% confidence limit.

Table 14.  Calculated microwave transitions in CS in order of frequency (MHz).

| Calculated Frequency | Isotopic Species | Transition J' - J" | (Est. Unc.) |
|---|---|---|---|
| 46247.472 | $^{13}C^{32}S$ | 1 - 0 | (0.040) |
| 48206.946 | $^{12}C^{34}S$ | 1 - 0 | (0.022) |
| 48586.5197[a] | $^{12}C^{33}S$ | 1 - 0 | (0.0248) |
| 48990.988 | $^{12}C^{32}S$ | 1 - 0 | (0.020) |
| 92494.084 | $^{13}C^{32}S$ | 2 - 1 | (0.081) |
| 96412.962 | $^{12}C^{34}S$ | 2 - 1 | (0.028) |
| 97172.090[a] | $^{12}C^{33}S$ | 2 - 1 | (0.056) |
| 97981.011 | $^{12}C^{32}S$ | 2 - 1 | (0.032) |
| 138738.97 | $^{13}C^{32}S$ | 3 - 2 | (0.13) |
| 144617.116 | $^{12}C^{34}S$ | 3 - 2 | (0.032) |
| 145755.760[a] | $^{12}C^{33}S$ | 3 - 2 | (0.130) |
| 146969.102 | $^{12}C^{32}S$ | 3 - 2 | (0.050) |
| 184981.28 | $^{13}C^{32}S$ | 4 - 3 | (0.20) |
| 192818.48 | $^{12}C^{34}S$ | 4 - 3 | (0.11) |
| 194336.58[a] | $^{12}C^{33}S$ | 4 - 3 | (0.29) |
| 195954.30 | $^{12}C^{32}S$ | 4 - 3 | (0.11) |
| 231220.15 | $^{13}C^{32}S$ | 5 - 4 | (0.31) |
| 241016.12 | $^{12}C^{34}S$ | 5 - 4 | (0.28) |
| 242913.61[c] | $^{12}C^{33}S$ | 5 - 4 | (0.55) |
| 244935.63 | $^{12}C^{32}S$ | 5 - 4 | (0.23) |
| 277454.72 | $^{13}C^{32}S$ | 6 - 5 | (0.49) |
| 289209.11 | $^{12}C^{34}S$ | 6 - 5 | (0.53) |
| 291485.88[a] | $^{12}C^{33}S$ | 6 - 5 | (0.95) |
| 293912.13 | $^{12}C^{32}S$ | 6 - 5 | (0.42) |

[a]Calculated hypothetical rotational transition frequency. See table 11 for transition frequencies including the hyperfine splittings.

### 3.3. CS References

#### a. Laboratory References

[53A] Bird, G. R., and Mockler, R. C., "The Microwave Spectrum of the Unstable Molecule Carbon Monosulfide", Phys. Rev. **91**, 222A (1953).

[55A] Mockler, R. C., and Bird, G. R., "Microwave Spectrum of Carbon Monosulfide", Phys. Rev. **98**, 1837 (1955).

[58A] Hurle, I. R., and Sugden, T. M., "Microwave Spectrometer for Study of Free Radicals", J. Sci. Instr. **35**, 319 (1958).

[63A] Kewley, R., Sastry, K. V. L. N., Winnewisser, M., and Gordy, W., "Millimeter Wave Spectroscopy of Unstable Species. I. Carbon Monosulfide", J. Chem. Phys. **39**, 2856 (1963).

[68A] Winnewisser, G., and Cook, R. L., "The Dipole Moment of Carbon Monosulfide", J. Mol. Spectrosc. **28**, 266 (1968).

[68B] Bates, H. E., Gallagher, J. J., and Derr, V. E., "Millimeter Interferometry of Unstable Molecules: Zeeman Effect in Carbon Monosulfide", J. Appl. Phys. **39**, 3218 (1968).

[70A] Gustafson, S., and Gordy, W., "Magnetic-Susceptibility Anisotropy of CO and CS", J. Chem. Phys. **52**, 579 (1970).

[70B] Silvers, S. J., Bergeman, T. H. and Klemperer, W., "Level Crossing and Double Resonance on the $A\,^1\Pi$ State of CS", J. Chem. Phys. **52**, 4385 (1970).

[71A] Field, R. W., and Bergeman, T. H., "Radio-Frequency Spectroscopy and Perturbation Analysis in CS $A\,^1\Pi$ ($v=0$)", J. Chem. Phys. **54**, 2936 (1971).

#### b. Interstellar References

Penzias, A. A., Solomon, P. M., Wilson, R. W., and Jefferts, K. B., "Interstellar Carbon Monosulfide", Astrophys. J. **168**, L53 (1971).

Wilson, R. W., Solomon, P. M., Penzias, A. A., and Jefferts, K. B., "Millimeter Observations of CO, CN, and CS Emission from IRC + 10216", Astrophys. J. **169**, L35 (1971).

Zuckerman, B., Morris, M., Palmer, P., and Turner, B. E., "Observations of CS, HCN, U89.2, and U90.7 in NGC 2264", Astrophys. J. **173**, L125 (1972).

Turner, B. E., Zuckerman, B., Palmer, P., and Morris, M., "Interstellar CS: Observations of New Transitions and Isotopic Species and a Study of Its Excitation.", Astrophys. J. **186**, 123 (1973).

### 4. Silicon Monoxide

The reanalysis of SiO was carried out in two fashions. Both methods employ $Y_{02}$ ($D_0$) calculated according to eq (4) with $\omega_e = 1241.4$ cm$^{-1}$ [52A], since only the $J = 1 \leftarrow 0$ transitions have been measured. The first calculation followed that discussed for several of the CO and CS isotopic species, whereby eq (6) was used with the $J = 1 \leftarrow 0$, $v = 0$ measured frequencies. In addition, since the Born-Oppenheimer approximation appears to hold to the accuracy of these measurements, all these isotopic forms of SiO were fit simultaneously by means of the isotope relations in eq (3). The second procedure, which was used for the final calculations reported in tables 15 to 19, followed the method described above, but also included the measured $^{28}Si^{16}O\ J = 1 \leftarrow 0$ transitions for the excited vibrational states. The results from both methods were in good agreement. The second method was selected for the final results, since it accounts for all the data available. The reanalysis given in table 15 produced nearly identical results to those reported by Törring [68A]. One minor difference occurs in the $Y_{02}$ ($D_0$) values employed, but the difference is well within the estimated uncertainties.

The estimated uncertainties were based on assuming a 1 percent model error in eq (4), used in deriving $Y_{02}$, to be equivalent to one standard deviation. Since all transitions were measured with equivalent accuracy, the fitting was carried out with uniform weighting. All constants and predicted transitions are reported with three standard deviation uncertainties in an attempt to estimate the 90 percent confidence limit.

### 4.1. Organization of the Spectral Tables

Tables 16, 17, and 18 contain the observed and predicted rotational transition frequencies of SiO. Since the table format is identical to those of CO and CS, refer to sections 2.2 and 3.2 for a complete description. Table 19 contains the SiO transition frequencies ordered according to increasing frequency.

### 4.2. Silicon Monoxide Spectral Tables

Table 15. Molecular constants for Silicon Monoxide.

| | $^{28}Si^{16}O$ | $^{29}Si^{16}O$ | $^{30}Si^{16}O$ | Ref. |
|---|---|---|---|---|
| $Y_{01}$ [MHz] | 21787.459(75) | 21514.070(75) | 21259.479(75) | a |
| $Y_{11}$ [MHz] | -151.048(114) | -148.214(114) | -145.591(114) | a |
| $Y_{21}$ [MHz] | 0.0762(30) | 0.0743(30) | 0.0726(30) | a |
| $Y_{02}(\equiv -D_e)$[kHz] | -29.87(30) | -29.113(30) | -28.44(30) | b |
| $\mu_0$ [D] | 3.0982(10) | | | 70A |

[a] Refit to data from [68A] with 3 standard deviation errors quoted. The present results are nearly identical to those in [68A].

[b] Calculated from $\omega_e = 1241.4_4$ cm$^{-1}$ [52A] using Kratzer's relation.

Table 16. The microwave spectrum of $^{28}Si^{16}O$ (MHz).

| Transition Upper State J' | – | Lower State J" | Vib. State v | Observed Frequency (Est. Unc.) | Calculated Frequency[a] (Est. Unc.) | Energy Levels in cm$^{-1}$ Upper State | Ref. |
|---|---|---|---|---|---|---|---|
| 1 | – | 0 | 0 | 43423.76(10) | 43423.788(78) | 1.448 | 68A |
| 1 | – | 0 | 1 | 43122.03(10) | 43121.998(99) | 1231.0 | 68A |
| 1 | – | 0 | 2 | 42820.48(10) | 42820.510(99) | 2448.8 | 68A |
| 1 | – | 0 | 3 | 42519.34(10) | 42519.328(131) | 3654.7 | 68A |
| 2 | – | 1 | 0 | | 86846.859(182) | 4.345 | |
| 3 | – | 2 | 0 | | 130268.49(32) | 8.690 | |
| 4 | – | 3 | 0 | | 173687.98(53) | 14.484 | |
| 5 | – | 4 | 0 | | 217104.61(83) | 21.726 | |
| 6 | – | 5 | 0 | | 260517.64(117) | 30.416 | |
| 7 | – | 6 | 0 | | 303926.37(175) | 40.554 | |

[a] The estimated uncertainty is 3 standard deviations, in an attempt to estimate the 90% confidence limit.

Table 17. The microwave spectrum of $^{29}Si^{16}O$ in the ground vibrational state (MHz).

| Transition Upper State J' | – | Lower State J" | Observed Frequency (Est. Unc.) | Calculated Frequency[a] (Est. Unc.) | Energy Levels in cm$^{-1}$ Upper State | Ref. |
|---|---|---|---|---|---|---|
| 1 | – | 0 | 42879.82(10) | 42879.846(78) | 1.430 | 68A |
| 2 | – | 1 | | 85758.997(180) | 4.291 | |
| 3 | – | 2 | | 128636.74(32) | 8.582 | |
| 4 | – | 3 | | 171512.40(53) | 14.308 | |
| 5 | – | 4 | | 214385.26(83) | 21.454 | |
| 6 | – | 5 | | 257254.61(117) | 30.035 | |
| 7 | – | 6 | | 300119.77(175) | 40.046 | |

[a] The estimated uncertainty is 3 standard deviations, in attempt to estimate the 90% confidence limit.

Table 18.  The microwave spectrum of $^{30}Si^{16}O$ in the ground vibrational state (MHz).

| Transition | | Observed Frequency | Calculated Frequency[a] | Energy Levels in cm$^{-1}$ | Ref. |
|---|---|---|---|---|---|
| Upper State J' | Lower State J" | (Est. Unc.) | (Est. Unc.) | Upper State | |
| 1 | 0 | 42373.34(10) | 42373.290(77) | 1.413 | 68A |
| 2 | 1 | | 84745.898(179) | 4.240 | |
| 3 | 2 | | 127117.14(32) | 8.480 | |
| 4 | 3 | | 169486.33(53) | 14.134 | |
| 5 | 4 | | 211852.79(83) | 21.201 | |
| 6 | 5 | | 254215.86(117) | 29.680 | |
| 7 | 6 | | 296574.80(175) | 39.573 | |

[a]The estimated uncertainty is 3 standard deviations, in an attempt to estimate the 90% confidence limit.

Table 19.  Calculated microwave transitions in SiO

in order of frequency (MHz)

| Calculated Frequency[a] | Isotopic Species | Transition J' - J" | Estimated Uncertainty |
|---|---|---|---|
| 42373.290 | $^{30}Si^{16}O$ | 1 - 0 | (0.077) |
| 42879.846 | $^{29}Si^{16}O$ | 1 - 0 | (0.078) |
| 43423.788 | $^{28}Si^{16}O$ | 1 - 0 | (0.078) |
| 84745.898 | $^{30}Si^{16}O$ | 2 - 1 | (0.179) |
| 85758.997 | $^{29}Si^{16}O$ | 2 - 1 | (0.180) |
| 86846.859 | $^{28}Si^{16}O$ | 2 - 1 | (0.182) |
| 127117.14 | $^{30}Si^{16}O$ | 3 - 2 | (0.32) |
| 128636.74 | $^{29}Si^{16}O$ | 3 - 2 | (0.32) |
| 130268.49 | $^{28}Si^{16}O$ | 3 - 2 | (0.32) |
| 169486.33 | $^{30}Si^{16}O$ | 4 - 3 | (0.53) |
| 171512.40 | $^{29}Si^{16}O$ | 4 - 3 | (0.53) |
| 173687.98 | $^{28}Si^{16}O$ | 4 - 3 | (0.53) |
| 211852.79 | $^{30}Si^{16}O$ | 5 - 4 | (0.83) |
| 214385.25 | $^{29}Si^{16}O$ | 5 - 4 | (0.83) |
| 217104.61 | $^{28}Si^{16}O$ | 5 - 4 | (0.83) |
| 254215.86 | $^{30}Si^{16}O$ | 6 - 5 | (1.17) |
| 257254.61 | $^{29}Si^{16}O$ | 6 - 5 | (1.17) |
| 260517.64 | $^{28}Si^{16}O$ | 6 - 5 | (1.17) |
| 296574.80 | $^{30}Si^{16}O$ | 7 - 6 | (1.75) |
| 300119.77 | $^{29}Si^{16}O$ | 7 - 6 | (1.75) |
| 303926.37 | $^{28}Si^{16}O$ | 7 - 6 | (1.75) |

[a]Only the transitions for SiO in the ground vibrational state are included although 3 transitions of $^{28}Si^{16}O$ in excited vibrational states are in the analysis.

## 4.3. SiO References

### a. Laboratory References

[52A] Lagerqvist, A., and Uhler, U., "The Ultra-violet Band-system of Silicon Monoxide", Ark. Fys. 6, 95 (1952).

[68A] Törring, T., "Das Mikrowellenrotationsspektrum des SiO", Z. Naturforsch. 23a, 777 (1968).

[70A] Raymonda, J. W., Muenter, J. S., and Klemperer, W. A., "Electric Dipole Moment of SiO and GeO", J. Chem. Phys. 52, 3458 (1970).

### b. Interstellar References

Wilson, R. W., Penzais, A. A., Jefferts, K. B., Kutner, M., and Thaddeus, P., "Discovery of Interstellar Silicon Monoxide", Astrophys. J. 167, L97 (1971).

Dickinson, D. F., and Gottlieb, C. A., "Comments on the Excitation and Abundance of Interstellar SiO, Based on a Search at 87 GHz", Astrophys. Lett. 7, 205 (1971).

Dickinson, D. F., "Detection of Silicon Monoxide at 87 GHz", Astrophys. J. 175, L43 (1972).